knowledge of the crystal system and the nature and directions of the symmetry axes. Thus, a transformation matrix to a basis which is most convenient for the study that is being carried out can always be obtained.

The lattice approach (FIG. **12**) obtains a transformation matrix from a skewed cell to a standard cell by analyzing the symmetry of the lattice. Each symmetry matrix Hs is used directly to calculate the nature of the symmetry axis and the direction of the axis with respect to the lattice. After the proper three directions for the standard cell edges have been chosen (step **1100**) as described hereinbelow, the task of obtaining a transformation matrix becomes a change-of-basis problem in linear algebra. That is, a skewed basis is to be transformed into a new standard basis. The first step (step **1200**) in solving this change of basis problem is to assemble an augmented matrix of lattice symmetry directions, where the directions are written as columns. The three symmetry directions chosen for the cell edges will be the first three columns in the augmented matrix and should be assembled with account taken of certain crystallograhic conventions. These include the definition of a right-handed coordinate system and observation of the preferred order of the axes. As summarized below, a transformation matrix from a skewed to a standard cell is found by applying elementary row operations to the augmented matrix until a new standard basis is obtained (step **1300**):

skewed basis	symmetry directions (optional)	100 010 001	→

new basis	symmetry directions (new basis)	transformation matrix

The new basis can be any 3×3 matrix. However, when determining a transformation matrix to a conventional unit cell, the new basis is usually the identity matrix and the mathematical operation involved is simply the taking of the inverse of a 3×3 matrix by reducing an augmented matrix to row echelon form. The choice of basis influences the relationships between the remaining vectors as well as the interpretation of the last three columns to give a transformation matrix. This is especially true for centered lattices and for the rhombohedral system. Although many variations are possible owing to the many bases that can be chosen, the relationships between the vectors is well defined and, in practice, the determination of a transformation matrix is straightforward for all cases. The lattice approach may be viewed as one form of lattice or cell reduction based on symmetry.

Because the symmetry matrices are generated by relating a cell to itself, the symmetry operations of the lattice are obtained. However, symmetry is often described in terms of equivalent positions for objects. This is the basis used for the object approach (FIG. **13**). As explained hereinabove with respect to Laue symmetry, the matrices Hs may be viewed as matrix representations of equivalent (h,k,l)'s. Therefore, in order to shift the emphasis from lattices or intensities (h,k,l)'s to objects or (x,y,z)'s, the nature and directions of the symmetry axes are calculated (step **1000**) from the transposes of the inverses of the symmetry matrices, $(Hs^{-1})^t$, and the three directions for the cell edges are chosen (step **1100**) as described hereinbelow. With this approach, the task of obtaining a transformation matrix is greatly simplified because the standard basis is the identity matrix and the standard matrix for a matrix transformation is the matrix itself. This means that the transformation matrix from any skewed cell to a conventional cell is obtained directly by making the three directions chosen for the cell edges rows in a matrix (step **1400**). As in the case of the lattice approach, the transformation matrix should be assembled so that the crystallographic conventions are met. The type of centering present is defined by a value for the determinant of the transformation matrix, except in orthorhombic systems where additional information is sometimes required.

Whether the lattice or the object approach is used to determine a transformation matrix to a standard cell, an important step is the selection of three linearly independent vectors in the proper directions to be used as directions for the cell edges (step **1100**). In the triclinic system, selection of cell edges is based on metric conditions. In the monoclinic system, the only symmetry direction, a two-fold axis, is labelled as b (the vectors a and c are chosen so that they lie in a plane perpendicular to b and meet additional metric constraints). The directions of the three two-fold axes in the orthorhombic system are selected for the cell edges. In the rhombohedral system, the directions for any two of the three two-fold axes and the direction of a three-fold axis are used as directions for a, b, and c, respectively. The resulting transformation may give either metrically rhomohedral or metrically hexagonal axes depending on the relationships between these vectors, i.e., the basis chosen. In the tetragonal system, the directions for two of five possible two-fold axes are taken as the a and b axes while the direction of a four-fold axis is selected for the c axis. Similarly, in the hexagonal system, directions for two of the seven two-fold axes are selected for a and b and the direction of a six-fold axis is selected for c. The cell edges for the cubic system are taken along three linearly independent four-fold axes. Thus, when choosing three symmetry directions to be used as cell edges, only the tetragonal and hexagonal crystal systems appear to allow more than one possibility.

The analysis-of-dependency-equations approach to choosing the directions to be used as cell edges will now be described with reference to FIG. **14**. In the tetragonal system, five of the matrices correspond to two-fold axes. Since one of these five axes is parallel to a four-fold axis, there are at most six combinations of two-fold axes to be considered. Likewise, in the hexagonal system, one of seven two-fold axes is parallel to a six-fold axis, leading to at most fifteen ways to choose two of the remaining six directions.

The first step (step **1110**) in the dependency equation procedure is to pick any two of the possible two-fold axes and arbitrarily assign these as the directions for the a and b axes. The direction used for the c axis is that of a four-fold axis in the tetragonal system and a six-fold axis for the hexagonal system. Next (step **1120**), a matrix is generated by making the symmetry directions columns, with the first three columns representing the a, b, and c directions. Using elementary row operations, the matrix is then reduced (step **1130**) to row echelon form. This step gives the dependency equations for the remaining symmetry directions with respect to the basis directions chosen.